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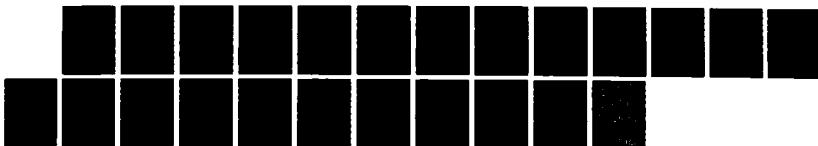
THE ANALYSIS OF MULTIRESPONSE EXPERIMENTS: A REVIEW(U)
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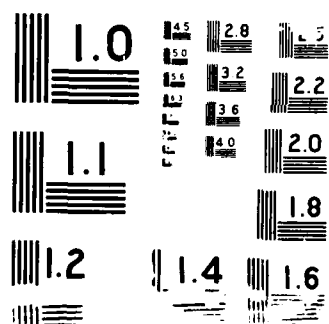
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The purpose of this article is to present an expository review of the literature on the analysis of multiresponse experiments. This covers multiresponse estimation, hypothesis testing, multiresponse designs, and multiresponse optimization. K. g.		

THE ANALYSIS OF MULTIRESPONSE EXPERIMENTS: A REVIEW

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1. INTRODUCTION

In many experiments it is not uncommon to have measurements on more than one response at a time. Such experiments are called multiresponse experiments. For the most part, response surface methodology has in the past dealt with single responses. The design and analysis of multiple responses received little attention in the statistical literature. This contrasts sharply with the growing need in science and industry to analyze multiresponse data. With the recent advances in modern technology it is becoming commonplace to obtain data that describe different facets of a system or a product. It is, therefore, imperative that practical multiresponse techniques be made available to researchers and data analysts.

When several responses are considered simultaneously, an investigation of one response should not be carried out independently of the other responses. This is particularly true when the responses are correlated. In parameter estimation, for example, relevant information from all the responses should be combined to estimate the parameters of the associated models, especially when some models contain common parameters. The same strategy applies to inference making concerning these parameters. It is also conceivable that the choice of a design in a multiresponse situation be governed by criteria that pertain to all the responses. Otherwise, a design suitable for one response may result in undesirable settings for the other responses. Similar remarks can be made with regard to multiresponse optimization. Optimum operating conditions must be determined with the wholeness of the responses put into proper perspective. If this is not properly done, then optimal conditions for one response may be far from optimal or even physically impractical for the remaining responses. Optimization is perhaps the most sought-after aspect of multiresponse analysis. It has many useful applications, particularly in product development. Hill and Hunter (1966) were among the

first to recognize its importance in the chemical industry.

The purpose of this chapter is to present an expository review of the literature on multiresponse analysis. The next six sections are organized as follows. In Section 2 methods of parameter estimation for a multiresponse model are reviewed. Some inference making procedures are mentioned in Section 3. The choice of a multiresponse design is discussed in Section 4. The problem of multiresponse optimization is treated in Section 5. Applications of multiresponse analysis are given in Section 6. Finally, in Section 7 comments and suggestions are made with regard to future research directions in multiresponse surface methodology.

2. MULTIRESPONSE PARAMETER ESTIMATION

The general multiresponse model is of the form

$$y_{ui} = \mathcal{F}_i(\mathbf{x}_u, \boldsymbol{\beta}) + \epsilon_{ui}, \quad u = 1, 2, \dots, N; \quad i = 1, 2, \dots, r, \quad (2.1)$$

where y_{ui} is the i^{th} response value at the u^{th} experimental run; \mathcal{F}_i is a model function, nonlinear in general, for the i^{th} response; $\mathbf{x}_u = (x_{u1}, x_{u2}, \dots, x_{uk})'$ is a vector of design settings for k input variables at the u^{th} experimental run; $\boldsymbol{\beta}$ is a vector of p unknown parameters; and ϵ_{ui} is a random error associated with y_{ui} . Let \mathbf{y}_i and $\boldsymbol{\epsilon}_i$ denote, respectively, the vectors of the i^{th} response values and corresponding random errors ($i = 1, 2, \dots, r$). The model in (2.1) can then be written as

$$\mathbf{Y} = \mathbf{F}(\mathbf{D}, \boldsymbol{\beta}) + \boldsymbol{\epsilon}, \quad (2.2)$$

[3]

where $\underline{Y} = [y_1 : y_2 : \dots : y_r]$, $F(\underline{D}, \underline{\beta})$ is an $N \times r$ matrix whose $(u, i)^{th}$ element is $F_i(x_u, \underline{\beta})$, and $\underline{\epsilon} = [\epsilon_1 : \epsilon_2 : \dots : \epsilon_r]$. In (2.2), \underline{D} denotes the $N \times k$ matrix of design settings for the input variables, x_1, x_2, \dots, x_k . It is assumed that the rows of $\underline{\epsilon}$ are independently distributed as $N(0, \underline{\Sigma})$, where

$$\underline{\Sigma} = (\sigma_{ij}) \quad (2.3)$$

is an unknown variance-covariance matrix for the r responses.

A method for estimating the elements of $\underline{\beta}$, which does not require knowledge of $\underline{\Sigma}$, was first introduced by Box and Draper (1965). The method calls for the minimization of the determinant $|\underline{S}(\underline{D}, \underline{\beta})|$ with respect to $\underline{\beta}$, where

$$\underline{S}(\underline{D}, \underline{\beta}) = [\underline{Y} - F(\underline{D}, \underline{\beta})]' [\underline{Y} - F(\underline{D}, \underline{\beta})]. \quad (2.4)$$

A Bayesian argument was used in the development of this method. The same result can also be achieved by using a maximum likelihood argument (see Bard, 1974, § 4.9, and Bates and Watts, 1985). I shall refer to this method as the Box-Draper Estimation Criterion. The resulting estimator, denoted by $\hat{\underline{\beta}}$, is therefore the maximum likelihood estimator of $\underline{\beta}$ under the assumption of normality made earlier. The maximum likelihood estimator of $\underline{\Sigma}$ is given by

$$\hat{\underline{\Sigma}} = \underline{S}(\underline{D}, \hat{\underline{\beta}})/N. \quad (2.5)$$

Box et al. (1970) extended the Box-Draper Estimation Criterion to situations with missing multiresponse data. The missing data were treated as additional parameters. Box (1971) proposed an alternative criterion that is more practicable when there are many missing values. Another approach was followed by Stewart and Sorensen (1981) who considered only the actually observed response values in the construction of the likelihood function. More recently, Stewart (1987) introduced modifications of the formulae for multiresponse parameter estimation, which apply to both missing and no missing data situations. A computational algorithm for the implementation of the Box-Draper Estimation Criterion was discussed by Bates and Watts (1984, 1987).

The existence of linear relationships among the responses can render meaningless the application of the Box-Draper Estimation Criterion. This is true by the fact that, when the responses are linearly related, the determinant of the positive semidefinite matrix $S(D, \beta)$ in (2.4) will attain its minimum value, namely zero, for all values of β . Such relationships usually occur as a consequence of some physical or chemical laws and are called stoichiometric (see Box et al., 1973). The presence of rounding errors in the responses can complicate the detection of these relationships since $|S(D, \beta)|$ will not exactly be equal to zero. This problem was addressed by Box et al. (1973) who proposed an eigenvalue analysis based on the observed multiresponse data. Further improvement to this eigenvalue analysis was proposed by Khuri and Conlon (1981) who also suggested a procedure for dropping responses that are linear functions of others. McLean et al. (1979) extended the work of Box et al. (1973) by discussing two additional cases that can cause problems when using the Box-Draper Estimation Criterion. Khuri (1987) pointed out that the implementation of the eigenvalue analysis can be adversely affected by differences in the responses' units of measurement and/or by large differences in

their orders of magnitude. He proposed scaling the responses before applying the Box-Draper Estimation Criterion.

Little is known about the statistical properties of Box and Draper's (1965) estimators. Being maximum likelihood, these estimators have the usual asymptotic properties. The small-sample properties, however, of these estimators are unknown. Approximate confidence regions for the parameters were given in Bard (1974, Chapter 7), Bates and Watts (1985), and Stewart (1987). An approximate expression for the variance-covariance matrix of the parameter estimators was reported in Ziegel and Gorman (1980). There is, however, some disagreement among these authors about the number of degrees of freedom for the error term used in these approximations.

2.1 Parameter Estimation in Linear Multiresponse Models

A linear multiresponse model is a special case of the general multiresponse model given in (2.1). It has the form

$$y_i = X_i \beta_i + \epsilon_i, \quad i = 1, 2, \dots, r, \quad (2.6)$$

where X_i is of order $N \times p_i$ and rank p_i , and β_i is a vector of p_i parameters for the i^{th} response. If the parameter vectors do not have elements in common, then the number of elements of $\beta = [\beta_1' : \beta_2' : \dots : \beta_r']'$ is $p = \sum_{i=1}^r p_i$. The multiresponse model described in (2.6) is called the multiple design multivariate linear model (see McDonald, 1975; Roy and Srivastava, 1964; and Srivastava, 1967).

The Box-Draper Estimation Criterion can be applied to estimate the parameters in

(2.6). However, if there are no common parameters among the elements of the β_i ($i=1,2,\dots,r$), the use of this criterion may not be computationally feasible. This is particularly true when p , the total number of parameters, is large. In this case the minimization of the determinant of $S(D, \beta)$ in (2.4), which is a complicated nonlinear function, can be an extremely difficult task.

An alternative estimation procedure is based on the Seemingly Unrelated Regression (SUR) approach. Numerous articles have been written on this subject since it was first introduced by Zellner (1962). In this approach, the models given in (2.6) are expressed as a single linear model of the form

$$\underline{y} = \underline{X}\underline{\beta} + \underline{\delta}, \quad (2.7)$$

where $\underline{y} = [y'_1 : y'_2 : \dots : y'_r]'$, $\underline{X} = \text{diag}(X_1 : X_2 : \dots : X_r)$, and $\underline{\delta} = [\epsilon'_1 : \epsilon'_2 : \dots : \epsilon'_r]'$.

The variance-covariance matrix of $\underline{\delta}$ is given by the direct product, $\underline{\Sigma} \otimes \underline{I}_N$, where $\underline{\Sigma}$ is the variance-covariance matrix for the r responses. The best linear unbiased estimator of $\underline{\beta}$ is

$$\tilde{\underline{\beta}} = (\underline{X}'\underline{\Delta}^{-1}\underline{X})^{-1}\underline{X}'\underline{\Delta}^{-1}\underline{y}, \quad (2.8)$$

where $\underline{\Delta} = \underline{\Sigma} \otimes \underline{I}_N$. Since $\underline{\Sigma}$ is unknown, an estimate must be provided. Zellner (1962) suggested the estimate, $\tilde{\underline{\Sigma}} = (\tilde{\sigma}_{ij})$, where

$$\tilde{\sigma}_{ij} = y'_i \left[\underline{I}_N - X_i(X'_i X_i)^{-1} X'_i \right] \left[\underline{I}_N - X_j(X'_j X_j)^{-1} X'_j \right] y_j / N, \quad i, j = 1, 2, \dots, r. \quad (2.9)$$

As can be noted from (2.9), this estimate is computed from the residual vectors, which result

from an ordinary least squares fit of the i^{th} and j^{th} single-response models. Using $\tilde{\Sigma}$ in (2.8), an estimate of $\underline{\beta}$, denoted by $\underline{\beta}^*$, can be obtained. This is usually referred to as the two-stage Aitken estimate. Other possible estimates of Σ were given in Srivastava and Giles (1987), where an exhaustive review of the SUR approach, including a listing of the statistical properties of $\underline{\beta}^*$, can be found.

In particular, if $X_i = X_0$ for all i , then

$$\tilde{\beta}_i = (X_0' X_0)^{-1} X_0' y_i. \quad (2.10)$$

We note that this estimate of $\tilde{\beta}_i$ does not depend on Σ . It can be shown that the $\tilde{\beta}_i$ ($i=1,2,\dots,r$) also satisfy the Box-Draper Estimation Criterion.

3. INFERENCE CONCERNING MULTIRESPONSE MODELS

Tests of hypothesis concerning estimable linear functions of the parameters for the multiple design multivariate linear model given in (2.6) are described in McDonald (1975). The tests are based on the union-intersection principle (Morrison, 1976, Chapters 4, 5), which leads to Roy's largest-root test statistic. Other multivariate tests can also be used. These include Wilks's likelihood ratio, Hotelling-Lawley's trace, and Pillai's trace. The percentage points of the test statistics are given in Roy et al. (1971) and in Seber (1984).

A multivariate lack of fit test was recently introduced by Khuri (1985). For this test, the linear multiresponse model is expressed in the form

$$Y = ZB + \epsilon, \quad (3.1)$$

where \underline{Y} and $\underline{\epsilon}$ are the same as in (2.2), $\underline{Z} = [\underline{X}_1 : \underline{X}_2 : \cdots : \underline{X}_r]$, and

$\underline{B} = \text{diag}(\underline{\beta}_1 : \underline{\beta}_2 : \cdots : \underline{\beta}_r)$. Model (3.1) is considered inadequate, or to suffer from lack of fit, if and only if the univariate model,

$$\underline{Y}\underline{c} = \underline{Z}\underline{B}\underline{c} + \underline{\epsilon}\underline{c}, \quad (3.2)$$

is inadequate for at least one \underline{c} . Here \underline{c} is a nonzero vector of arbitrary constants. By invoking the union-intersection principle, a multivariate lack of fit test can be developed using any of the four multivariate tests mentioned earlier. Thus, a significant multivariate lack of fit test indicates that there exists at least one linear combination of the responses that cannot be adequately represented by the same linear combination of the models in (2.6). Khuri (1985) proposed a procedure for identifying the responses, or subsets of the responses, that are influential contributors to lack of fit whenever the test is significant.

Comparisons among the parameter vectors from correlated response models were considered by several authors. The case of $r=2$ responses was addressed by Yates (1939). Zellner (1962) applied his test for aggregation bias to any number of responses. Both Yates and Zellner's tests, however, are approximate and require providing an estimate of the variance-covariance matrix $\underline{\Sigma}$. More recently, Smith and Choi (1982) developed an exact method for comparing two correlated models that does not require estimation of $\underline{\Sigma}$. An extension of this exact method to several correlated models was given by Khuri (1986).

4. MULTIRESPONSE DESIGN CRITERIA

The choice of a design for a multiresponse model requires more careful considerations

than in the single-response case. This is because a multiresponse design criterion must incorporate measures of efficiency that pertain to all the responses. Draper and Hunter (1966, 1967) used Bayesian arguments to develop design criteria for augmenting an existing design for parameter estimation with new experimental runs. Knowledge of the variance-covariance matrix, Σ , for the responses was assumed. Box and Draper (1972) presented a design criterion for the unknown Σ case that also allows for different variance-covariance structures for different blocks of the data.

Fedorov (1972) introduced a sequential procedure for the construction of a D-optimal design for a linear multiresponse model of the form given in (2.7). This procedure is based on a multivariate version of the Kiefer-Wolfowitz (1960) Equivalence Theorem, and requires knowledge of Σ . Recently, Wijesinha and Khuri (1987a) proposed a modification of Fedorov's procedure, which can be applied when Σ is not known.

Two other design criteria for a linear multiresponse model were presented in Wijesinha and Khuri (1987b). These are derived on the basis of maximizing the power of the multivariate lack of fit test discussed in Section 3. The two criteria are multivariate extensions of the Λ_1 and Λ_2 optimality criteria described in Jones and Mitchell (1978). A sequential procedure for the generation of Λ_2 -optimal designs was given in Wijesinha and Khuri (1987b).

Recently, Khuri (1988) extended the concept of rotatability to the multiresponse case. Multiresponse rotability conditions were developed in a manner similar to that of Box and Hunter (1957).

5. MULTIRESPONSE OPTIMIZATION

This is one area that clearly has many useful applications. In product development,

for example, it is of interest to determine optimum operating conditions that result in a product with desirable properties. In this case, the responses are measures of different attributes considered important in determining the quality of a product. It is, therefore, imperative that these responses be optimized simultaneously.

For quite some time, the problem of multiresponse optimization has remained not very well defined. One reason for this is the variety of ways in which multiresponse data can be ordered. A simple, and perhaps the oldest, approach to this problem is a graphical one based on superimposing response contours. By examining the region where the contours overlap, it is possible to arrive at conditions that are reasonably "good" for all the responses (see, for example, Lind et al. 1960). Obviously, this method has its limitations in the presence of many responses. It is also not very practical when the number of input variables exceeds three. Furthermore, no account is given of the random nature of the responses.

In the dual response system of Myers and Carter (1973), a "primary" response function is optimized subject to the condition that a "secondary" response assumes desirable values. The method used is similar to ridge analysis in the single-response case (Hoerl, 1959). Biles (1975) extended this method by considering several "secondary" response functions.

Harrington (1965) and Derringer and Suich (1980) adopted a different approach to multiresponse optimization. The multiresponse values are transformed using particular desirability functions. The choice of these functions is subjective and is governed by how the experimenter assesses the importance of each response. The individual desirability functions are combined into a single function, namely, their geometric mean, which serves as a measure of the overall desirability of the multiresponse system. Optimum conditions on the input variables can then be determined by maximizing the overall desirability function over the

experimental region.

Another optimization procedure was introduced by Khuri and Conlon (1981). This procedure applies to linear multiresponse models of the form (2.6), but with $X_1 = X_2 = \dots = X_r = X_0$. It is based on a simple geometric concept that has its roots in the superimposition of response contours approach mentioned earlier. To understand this concept, let ϕ_i denote the optimum value of $\hat{y}_i(x)$, the i^{th} predicted response function ($i=1,2,\dots,r$), over the experimental region. This optimum is obtained independently of the other responses. Let $\underline{\phi} = (\phi_1, \phi_2, \dots, \phi_r)'$. If all the ϕ_i ($i=1,2,\dots,r$) are attained at the same point in the experimental region, then an "ideal" optimum is said to be achieved. In practice, it is very rare that such an optimum occurs. Deviations from the "ideal" optimum can therefore be measured by a distance function, $\rho[\underline{\hat{y}}(x), \underline{\phi}]$, where $\underline{\hat{y}}(x)$ is the vector of r predicted response functions. By minimizing this distance function, "compromise" conditions that are somewhat favorable to all the responses can be obtained. Several options are available for the distance function ρ depending on the nature of the variance-covariance matrix, Σ , for the responses. One option takes into account the variability of the random vector $\underline{\phi}$. More details about this can also be found in Khuri and Cornell (1987, Chapter 7). Unlike the other optimization procedures, this one takes into consideration correlations among the responses as well as their individual variances. It also provides safeguards against sizable variations associated with the estimated optima.

6. APPLICATIONS

The development of multiresponse analysis has been lagging in comparison with its single-response counterpart. It is fair to say that the deployment of the available multiresponse techniques has also been limited. This can be attributed to several factors.

First, the subject area is fairly new, developed only in the last two decades. There is always a "lag time" after a technique is introduced in the statistical literature and before it is adopted by the user. Second, the needed software for analyzing multiresponse data is practically nonexistent. Since multiresponse techniques are generally more involved than in the single-response case, lack of software can be detrimental to their use. As a result, and because the software for analyzing a single response is readily available, one is always tempted to apply separate analyses to the individual responses. This, however, can cause the analysis of multiresponse experiments to be woefully inadequate. Third, statistical researchers have not "campaigned" hard enough to convince potential subject matter users of the utility of the multiresponse approach.

In this section, reference will be made to some articles in which multiresponse experiments were described. No attempt, however, was made at presenting an exhaustive survey. The purpose of the cited references is to give some examples that may help illustrate multiresponse applications.

In their review article, Hill and Hunter (1966) included a section on multiresponse applications. One of these applications was a demonstration by Lind et al. (1960) of the determination of optimum operating conditions by superimposing response contours. The responses of interest were the cost and yield of a certain antibiotic. The objective was to establish the levels of the complexing agents (the process input variables) that increased the yield by 5% and reduced the cost by \$5.00 per kilogram of product.

The majority of the more recent articles on multiresponse analysis emphasize the estimation aspect using the Box-Draper Estimation Criterion. Ziegel and Gorman (1980) discussed applications of this criterion in fitting kinetic reaction models. They also

demonstrated the utility of using the multiresponse approach in getting a better understanding of the reaction mechanism, and a more comprehensive assessment of model adequacy. Bates and Watts (1985) obtained estimates of the parameters in a multiresponse system described by linear differential equations. McLean et al. (1979) presented an example from reaction kinetics to illustrate the importance of applying the eigenvalue analysis discussed in Section 2. Kemeny et al. (1982) discussed several parameter estimation methods based on different extensions of the Box-Draper Estimation Criterion.

Multiresponse parameter estimation was also discussed by Boag et al. (1976) using data from the vanadia-catalyzed gas-phase oxidation of o-xylene in a recirculation reactor. Foster et al. (1982) investigated the adequacy of two kinetic models that describe the oxidation of naphthalene over an industrial vanadium pentoxide catalyst.

The food industry has provided a good source of multiresponse data. Richert et al. (1974) investigated the effects of five input variables on several responses that describe the foaming properties of whey protein concentrates. Schmidt et al. (1979) studied the effects of cysteine and calcium chloride combinations on the textural characteristics of dialyzed whey protein concentrates gel systems. Ahmed et al. (1983) conducted a study for the purpose of developing acceptable fish patties from minced sheepshead flesh. The responses of interest measured the textural quality of the cooked patties. Tseo et al. (1983) applied Khuri and Colon's (1981) optimization procedure to determine optimum washing conditions for quality improvement of minced mullet flesh.

Prasad and Rao (1977) discussed the problem of model discrimination for a multiresponse system. They presented a sequential design strategy to achieve a better discrimination between rival models. Boag et al. (1978) applied the Draper-Hunter (1966)

design criterion to obtain additional experimental runs in a reaction network study. The study involved the vanadia-catalyzed oxidation of o-xylene in a recirculation reactor.

More examples of multiresponse experiments and applications can be found in the review article by Myers et al. (1988, in press).

7. FUTURE DIRECTIONS

As was mentioned earlier, multiresponse analysis is a relatively new field in response surface methodology. As such, it provides a fertile ground for new research development.

In the area of estimation, there is a need to have a better understanding of the small-sample properties of Box and Draper's (1965) estimators. Asymptotic results are not very useful in a response surface investigation, particularly in an industrial setting. It is to be remembered that one of the objectives of response surface methodology is the exploration of the response surface using a minimum number of experimental runs. The bias associated with these estimators is unknown and should be investigated. There is also a need to compare them with the SUR estimators mentioned in Section 2. Furthermore, there are no known diagnostic procedures that can help the user determine the adequacy of the fitted multiresponse model and/or detect failures of the assumptions when Box and Draper's (1965) estimates are used.

The design area is not well developed in the multiresponse case. Most of the known multiresponse design criteria are variance related relying mainly on D-optimality. Designs that reduce model bias are unknown. The Box-Draper (1959) design criterion has no analog for the multiple design multivariate linear model given in (2.6). Robust designs that protect against outliers or failure of the normality assumption need to be established.

The acute shortage of software is critical. Unless this problem is resolved, data analysts will, unfortunately, not be attracted to multiresponse techniques. A serious effort should therefore be made to alleviate the problem. This would require the cooperation of several research workers and data analysts.

Finally, there appears to be some need for multiresponse techniques that apply when some or all of the responses are qualitative. Multivariate extensions of generalized linear models (GLIM) may prove useful. As a matter of fact, this area is little developed in response surface methodology, even in the single-response case.

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